Radiative lifetimes of exited states in Mo II

P. Bogdanovich , I. Martinson[1] and H. Nilsson[1]

State Institute of Theoretical Physics and Astronomy
Goštauto 12, Vilnius 2600, Lithuania
Tel +370-2-620949, Fax +370-2-225361, E-mail: pavlas@mserv.itpa.lt,
[1] *Department of Physics, Lund University, SE-22100, Lund, Sweden*

Theoretical lifetimes of the levels belonging to the excited $4d^45p$ and $4d^35s5p$ configurations of Mo II were determined by *ab initio* calculations. They were performed using CI method in the basis of HF radial orbitals of the configurations under study and transformed radial orbitals with variable parameters (TRO) describing virtual excitations of the electrons in the admixed configurations. As shown in [1] and as follows from the recent Ag II and Au II lifetime calculations [2, 3] and other publications, TRO describe the solutions of MCHF equations very well. TRO for $5f$-, $6s$-,...,$6h$-, $7s$-,...,$7i$-, $8s$-,...,$8g$-, $9s$-,...$9g$-, $10s$-,...,$10g$-electrons were included into the basis set. Due to the known degeneracy of the energies of $4d$- and $5s$-electrons, first of all it is necessary to take into account CI of three configurations $4d^45p + 4d^35s5p + 4d^25s^25p$ for evaluation of the initial excited states. Each of these configurations was adjusted using its own particular set of the most important admixed configurations, generated by one- and two-electron virtual excitations from $4p$-, $4d$-, $5s$-, and $5p$-shells. Thus, a basis set including 44 admixed configurations was formed. The number of admixed configurations could be larger. However, the limited capacities of the personal computer allowed us to calculate and diagonalize matrices of the order no larger than 11000 for individual J values. The total number of terms of the admixed configurations taken into account was mainly determined by a very large number of such terms in important configurations obtained by virtually exciting one $4p$-electron to the state with $l = 3$. For instance, from the total number of terms of configuration $4p^54d^45s5p5f$ that equals 3693, we had to take into account 2196. The correlation corrections of the term energies due to the configurations possible in the given basis set, but not directly used for energy matrix calculations, were taken into account in the second order of the perturbation theory, as described in [4]. The correlation corrections for calculating the spectra of the three final configurations $4d^5 + 4d^45s + 4d^35s^2$ were taken into account in a similar way. The eigenfunctions obtained in these calculations were used to determine the probabilities of electronic transitions using two forms of the transition operator: length and velocity. The discrepancies between the lifetime values obtained using the two forms of the transition operator were less than 10 percents for most of the levels, which is quite an acceptable accuracy for the complex configurations studied in the present work.

[1] P. Bogdanovich and R. Karpuškiene, *Lithuanian Physics Journal* **39** 193 (1999).
[2] P. Bogdanovich and I. Martinson, *Physica Scripta* **60** 217 (1999).
[3] P. Bogdanovich and I. Martinson, *Physica Scripta* **61** 142 (2000).
[4] P. Bogdanovich *et al*, *Physica Scripta* **56** 230 (1997).